Sodium 3-nitrobenzenesulfonate

127-68-4 | DTXSID2027048

Model Performance

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Model	II)ata
IVIOGCI	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 48.0 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.30e-01

Confidence level: 7.61e-01

Nearest Neighbors from the Training Set

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Picloram

Measured: 20.0 Predicted: 27.1

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Clopyralid

Measured: 36.3 Predicted: 37.7

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Chloramben

Measured: 30.2 Predicted: 41.0

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3-Bromophenylurea Measured: 132 Predicted: 114 Image not found

N-(4-Bromophenyl)urea

Measured: 115 Predicted: 122